Compressible Flow Simulation on Roadrunner

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Turbulence is an inherently multiscale phenomenon, encompassing a large range of length and time scales, all of which must be resolved in a direct numerical simulation (DNS). The DNS technique also requires that the numerical errors remain small and not affect the solution. DNS allows a degree of control of specific physical phenomena not accessible in experiments, leading to improved understanding and, ultimately, to models for large multiphysics codes. However, the numerical requirements significantly restrict the range of accessible flows and parameters, as they require very large grids. Recent progress in computer hardware, based on heterogeneous architectures, could significantly advance our state-of-the-art turbulence simulations and, thus, turbulence theory and modeling.

The IBM Cell Broadband Engine (Cell BE) used in the Roadrunner supercomputer is an example of the newest generation of accelerators. Common to many of these architectures is the existence of multiple processing cores (synergistic processing units, or SPUs, in this case) with independent, high bandwidth access to local memory.

CFDNS is a Fortran-structured grid code that simulates the compressible Navier-Stokes equations in 3D. Multiple species are allowed, each with realistic material properties equation of state (EOS), as well as Cartesian, cylindrical, and spherical grid geometries. The bulk of the time in the code is spent in either computing the update equations or computing the derivatives of the various fields. The update equation is computed in a pointwise manner throughout the domain and is straightforward to vectorize once all the terms have been evaluated. The derivative step uses a compact finite difference (Pade) scheme that requires a tridiagonal inversion along the direction in which the derivative is being performed. Since the data is laid out in 3D, this requires a strided load of the data.

A subset of the base code was ported to the Cell BE architecture and implemented in C with SPU extensions. The derivative calculation vectorizes naturally in the x and y directions, since the data is contiguous in z. For the z derivative, the data must be reordered in local store for good performance, but is not reordered in main memory. Each SPU works on a different portion of the data and executes its own direct memory access (DMA) calls independently in order to maximize performance. Similar data partitioning is used for the update step.

The Cell BE implementation of the code was benchmarked against a functionally identical C code running on the Opteron. Significant speedups of 40X (64^3) to 50X (128^3) were observed. The primary benefit for the Cell BE implementation is the ability to independently access main memory, allowing an effective memory access rate of ~ 12 GB/s (50 percent of theoretical peak) [1].

A full parallel implementation of the code on the hybrid Roadrunner architecture [2] is currently in final testing, in anticipation of the full Roadrunner deployment, which will allow simulations at resolutions of 4096^3. These will be by far the largest compressible turbulence simulations ever performed, and we expect them to allow significant advancement on the theory and modeling of compressible turbulence. Targeted applications include Type 1a supernova and inertial-confinement fusion (ICF) modeling.

The parallel code exhibits speedup on the order of 20X (128^3 per node). Extensive reorganization of the code was required to achieve this speedup, to reduce internode data movement. The speed of the new code, combined with advances in graphics performance, makes 'live' visualization of evolving turbulent flows feasible in the near future (Fig. 1).

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[1] J. Mohd-Yusof, D. Livescu, M.R. Petersen, "Roadrunner: Compressible Turbulence Simulation" at SC07 (International Conference for High Performance Computing, Network, Storage and Analysis) (2007).
[2] J. Mohd-Yusof et al., "Simulation of Compressible Fluid Flow on Roadrunner" at *SC08* (International Conference for High Performance Computing, Network, Storage and Analysis) (2008).

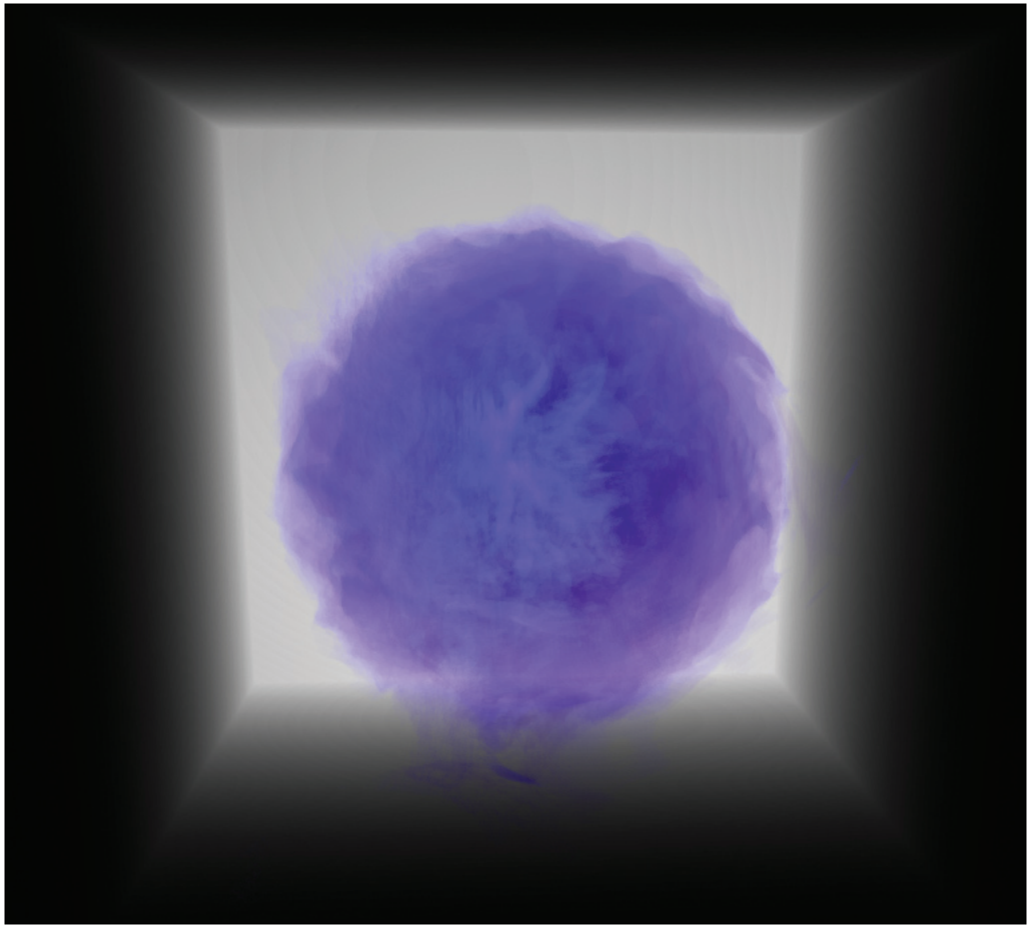

Fig. 1. Volume-rendering of scalar concentration from a test simulation using the Roadrunner code. The rendering is done using graphics processing unit (GPU)-accelerated custom code, which will eventually allow realtime visualization of turbulence simulation results. (Courtesy of Pat McCormick, CCS-1)

Funding Acknowledgments
- DOE, NNSA, Advanced Simulation and Computing Program Roadrunner Project
- LANL Directed Research and Development Program